

Investigation of the Finite Group Invariance of $T \otimes (e \oplus t_2)$ Jahn Teller System

Hayriye Tütüncüler, Umut Bora Türkdönmez and Ramazan Koç

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Abstract

Jahn-Teller (JT) interaction matrices are constructed for $T_1 \otimes (e \oplus t_2)$ JT systems for Octahedral group by using the symmetry properties. In chemical applications of JT effect, the shape of adiabatic potential near instability point is of primary importance. Analysis of adiabatic potential energy surface (APES) is made by introducing a new approach for this group. Group symmetry is broken into its little groups due to JT interaction. This problem is devoted to the determination of extremum points on the JT surface by breaking symmetries of group into its maximal little groups.